

Many-body interaction effects in doped and undoped graphene: Fermi liquid versus non-Fermi liquid

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We consider theoretically the electron-electron interaction induced many-body effects in undoped ('intrinsic') and doped ('extrinsic') 2D graphene layers. We find that (1) intrinsic graphene is a *marginal* Fermi liquid with the imaginary part of the self-energy, $\text{Im}\Sigma(\omega)$, going as linear in energy ω for small ω , implying that the quasiparticle spectral weight vanishes at the Dirac point as $(\ln\omega)^{-1}$; and, (2) extrinsic graphene is a well-defined Fermi liquid with $\text{Im}\Sigma(\omega) \sim \omega^2 \ln\omega$ near the Fermi surface similar to 2D carrier systems with parabolic energy dispersion. We provide analytical and numerical results for quasiparticle renormalization in graphene, concluding that all experimental graphene systems are ordinary 2D Fermi liquids since any doping automatically induces generic Fermi liquid behavior.

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Recent progress in the experimental realization of a single layer of graphene [1] has spawned tremendous interest and activity in studying the properties of this unique two-dimensional system. Graphene has a honeycomb real-space lattice structure, which comprises two interpenetrating triangular sublattices A and B, and a concomitant reciprocal space honeycomb structure with the hexagonal Brillouin zone cornering at the K points. At these so-called "Dirac points" the low-energy excitations satisfy the massless Dirac equation, and the bandstructure for the "Dirac fermions" is uniquely different from the "Schrödinger fermions" of the regular two-dimensional electron gas (2DEG), exhibiting a linear energy dispersion $\varepsilon_k = vk$ (having an effective "speed of light" $v \simeq 10^6 \text{ms}^{-1}$ [1]) with the conduction and valence bands connected at the Dirac point. 2D graphene is thus a rather unique chiral Dirac system. This apparently peculiar bandstructure of graphene is readily accounted for using a tight-binding model with nearest-neighbour hopping, where in the vicinity of the crossing of the energy dispersion relations for the two bands, the energy is linear with respect to the momentum [2]. In an exciting recent development, this linear dispersion has been directly observed using angle-resolved photoemission spectroscopic (ARPES) measurements [3]. Another recent ARPES experiment [4] finds that this linear spectrum manifests subtle many-body renormalization effects, preserving, however, the Landau Fermi liquid quasiparticle picture. On the theoretical side, there has been a number of works in the literature on the effects of electron-electron interaction in graphene [5, 6]; however, the consideration has been solely based on undoped graphene so far, and explicit analytical results for either the doped or the undoped case are still lacking. The recent ARPES experiments are in doped graphene, and we show in this paper that doped and undoped graphene have qualitatively different quasiparticle spectra.

In this paper, we critically address the question of

whether two-dimensional graphene is a Fermi liquid or not using the diagrammatic perturbation theory. We perform concrete theoretical calculations for the quasiparticle lifetime, renormalization factor, and effective velocity for both the doped and the undoped case. We find that extrinsic graphene manifests a Fermi liquid behavior similar to the regular 2DEG, indicating that the quasiparticle description is indeed valid as substantiated by the recent experiment [4]. For intrinsic (i.e. zero doping) graphene, we find that the quasiparticle lifetime scales linearly with energy ω above the Fermi energy (i.e. the Dirac point) and the renormalization factor at the Fermi energy vanishes, exhibiting a quintessential marginal Fermi liquid behavior.

Thus, the quasiparticle behavior of 2D graphene depends crucially on whether the system is doped or not: While undoped intrinsic graphene is a marginal Fermi liquid, doped graphene with free carriers is invariably a garden-variety 2D Fermi liquid. Since the presence of charged impurities in the substrate (i.e. unintentional dopants) would invariably induce *some* carriers even in nominally undoped graphene, we conclude that the generic behavior of 2D graphene is likely to be that of a 2D Fermi liquid.

The low-energy Hamiltonian for graphene is given by $H = v\boldsymbol{\sigma} \cdot \mathbf{k}$, where v is the Fermi velocity of the Dirac fermions, $\boldsymbol{\sigma}$ is the set of Pauli matrices representing the two (A and B) sublattice degrees of freedom (throughout this paper we choose $\hbar = 1$). This Hamiltonian describes a cone-like linear energy spectrum with conduction band energy dispersion vk and valence band energy dispersion $-vk$. The corresponding eigenstates are given respectively by the plane wave $|\mathbf{k}\rangle$ multiplied by the spinors $|\pm\rangle = [1 \pm e^{i\phi}]/\sqrt{2}$, where $\phi = \tan^{-1}(k_y/k_x)$ is the polar angle of the momentum \mathbf{k} . The Green function is given accordingly as $G_{\mathbf{k}}(ik_n) = G_{\mathbf{k}+}(ik_n)|+\rangle\langle+| + G_{\mathbf{k}-}(ik_n)|-\rangle\langle-|$, where the label \pm , also called the chirality, signifies the conduction band and valence band

respectively, and $G_{\mathbf{k}\pm}(ik_n) = 1/(ik_n \mp \varepsilon_k)$ is the Green function in the diagonal basis, where we have denoted $\varepsilon_k = vk$. The self-energy can also be similarly expressed as

$$\Sigma_{\mathbf{k}}(ik_n) = \Sigma_{\mathbf{k}+}(ik_n)|+\rangle\langle+| + \Sigma_{\mathbf{k}-}(ik_n)|-\rangle\langle-|, \quad (1)$$

where the leading-order self-energy in the diagonal basis is given by

$$\Sigma_{\mathbf{k}\pm}(ik_n) = -k_B T \sum_{\lambda=\pm} \sum_{\mathbf{q}, iq_n} \left[G_{\mathbf{k}+\mathbf{q}\lambda}(ik_n + iq_n) \frac{1 \pm \lambda \cos\theta}{2} V_{\mathbf{q}}/\epsilon(q, iq_n) \right], \quad (2)$$

with the Coulomb potential $V_{\mathbf{q}} = 2\pi e^2/q$, dielectric function ϵ and the scattering angle from \mathbf{k} to $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ denoted as θ . The factor $(1 \pm \cos\theta)/2$ comes from overlap of the eigenstates of the Hamiltonian H . Following standard procedure of analytic continuation, the retarded self-energy from Eq. (2) is obtained as

$$\Sigma_{\mathbf{k}\pm}^R(\varepsilon) = -\frac{1}{2} \sum_{\lambda=\pm} \sum_{\mathbf{q}} V_{\mathbf{q}}(1 \pm \lambda \cos\theta) \left\{ \text{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} n_B(\omega) \frac{\text{Im}[1/\epsilon(q, \omega + i0^+)]}{\varepsilon + \omega - \lambda \varepsilon_{\mathbf{k}+\mathbf{q}} + i0^+} + \frac{n_F(\lambda \varepsilon_{\mathbf{k}+\mathbf{q}})}{\epsilon(q, \lambda \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon - i0^+)} \right\}, \quad (3)$$

where n_F and n_B are the Fermi and Bose distribution functions, respectively, and P stands for principal value integration. In the following, we proceed to calculate the quasiparticle lifetime, renormalization factor and effective velocity at zero temperature for graphene in two distinct cases: extrinsic graphene with doping (Fermi energy $\varepsilon_F > 0$) and intrinsic graphene ($\varepsilon_F = 0$). Note that we calculate our self-energy (Fig. 1) in the leading-order infinite ring-diagram single-loop expansion approximation, which is essentially exact in the effective high-density regime of relevance to graphene. In fact, our self-energy calculation (Fig. 1) is a much better quantitative approximation to graphene than the so-called GW approximation in regular metals and semiconductors which are never in the high-density regime.

Extrinsic graphene. For extrinsic graphene, the quasiparticle is located in the vicinity of the Fermi level and we only need to consider the renormalized Fermi liquid parameters in the conduction band (or the valence band, depending on whether electrons or holes are the carriers as determined by doping). The lifetime of the quasiparticle $-1/2\tau_+$ is obtained from the imaginary part of the self-energy Eq. (3) within the on-shell approximation $\varepsilon = \varepsilon_k$:

$$\text{Im}\Sigma_{\mathbf{k}+}^R(\varepsilon_k) = \frac{1}{2} \sum_{\lambda=\pm} \sum_{\mathbf{q}} (1 + \lambda \cos\theta) V_{\mathbf{q}} [n_B(\lambda \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_k) + n_F(\lambda \varepsilon_{\mathbf{k}+\mathbf{q}})] \text{Im} \left[\frac{1}{\epsilon(q, \lambda \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_k + i0^+)} \right]. \quad (4)$$

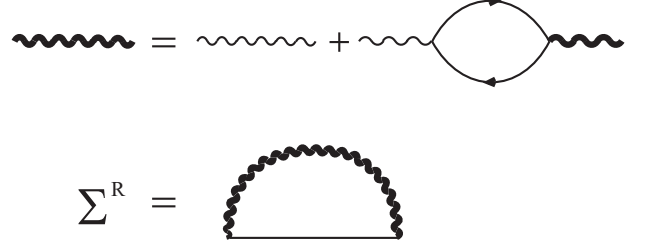


FIG. 1: The Feynman diagrams for the screened Coulomb interaction within the RPA, and the retarded self-energy Σ^R Eq. (2). The thin and thick wiggly lines denote respectively the bare and the RPA-screened interaction. The thin straight line stands for the bare Green function. This is the standard ring diagram approximation for self-energy exact in the $r_s \ll 1$ limit.

At zero temperature, it can be seen that interband scattering from the valence band $\lambda = -1$ vanishes in Eq. (4), and the expression reduces to (dropping the momentum \mathbf{k} and energy ε labels in the self-energy):

$$\text{Im}\Sigma_+^R = -\pi e^2 \int_0^{2\pi} d\theta (1 + \cos\theta) \int_{k_F}^k dk' k' \frac{\text{Im}[1/\epsilon(|\mathbf{k} - \mathbf{k}'|, \varepsilon_{k'} - \varepsilon_k + i0^+)]}{\sqrt{k^2 + k'^2 - 2kk'\cos\theta}}. \quad (5)$$

In order to maintain analytic tractability, we consider the long-wavelength $x = q/2k_F \ll 1$ limit and perform an analytical evaluation of the quasiparticle lifetime. For small x , the dominant contribution in Eq. (5) from the imaginary part of the dielectric function comes from low energies $u = \omega/vq \ll 1$, in which case the irreducible polarizability for graphene (in the doped regime) is given in the leading order by [7] $\Pi(q, \omega) \simeq \nu(1 + iu) + (q/4v)$, where $\nu = 4\varepsilon_F/2\pi v^2 = 2k_F/\pi v$ is the graphene density of states at the Fermi level. We employ the random phase approximation (RPA) (Fig. 1) for the screened Coulomb potential and calculate the dielectric function as $\epsilon(q, \omega)/\epsilon_m = 1 + V_q \Pi(q, \omega)$ (here ϵ_m is the background dielectric constant). Substituting this expression for the dielectric function in Eq. (5), we obtain

$$\text{Im}\Sigma_+^R = \frac{\pi e^2}{q_{\text{TF}}} \int_{k_F}^k dk' k' (k - k') \int_0^{2\pi} d\theta \frac{(1 + \cos\theta)}{\sqrt{k^2 + k'^2 - 2kk'\cos\theta}}, \quad (6)$$

where we have defined the Thomas-Fermi wavenumber as $q_{\text{TF}} = 4e^2 k_F / v \epsilon_m$. After carrying out the angular integral, expanding in the small parameter $\delta = k - k' \ll k_F$, and integrating over k' , we obtain

$$\text{Im}\Sigma_+^R = \frac{\xi_k^2}{8\pi \varepsilon_F} \left[\ln \left(\frac{\xi_k}{8\varepsilon_F} \right) + \frac{1}{2} \right], \quad (7)$$

where $\xi_k = \varepsilon_k - \varepsilon_F$ is the single-particle energy reckoned from the Fermi level. Comparing with the corresponding expression for the regular 2DEG [8] $\text{Im}\Sigma^R = (\xi_k^2/2\pi\varepsilon_F)[\ln(\xi_k/16\varepsilon_F) - 1/2]$, it is instructive to note that (1) the factor of two difference inside the logarithm comes from the linearity of the graphene spectrum; (2) the sign difference in the subleading term comes from the vanishing of the interband contribution from the valence band in Eq. (4) at zero temperature.

Next we consider the renormalization factor for the Dirac quasiparticle $Z = 1/(1 - A)$, where A is the derivative of the real part of the self-energy Eq. (2) with respect to energy:

$$A = -\frac{1}{2} \frac{\partial}{\partial \varepsilon} \text{Re} \sum_{\mathbf{q}, \lambda} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\mathbf{k}+\mathbf{q}\lambda}(ik_n + i\omega) (1 + \lambda \cos\theta) V_{\mathbf{q}}/\epsilon(q, i\omega) \Big|_{k, \varepsilon=k_F, \varepsilon_F}. \quad (8)$$

As usual, we perform the standard trick for evaluating the real part of the retarded self-energy by decomposing Eq. (8) into line and pole contributions [9] and performing analytic continuation $ik_n \rightarrow \varepsilon + i0^+$, and then integrating by parts the ω -integral [10], obtaining

$$A = \frac{1}{\pi} \text{Im} \sum_{\mathbf{q}, \lambda} \int_0^{\infty} d\omega G_{\mathbf{k}+\mathbf{q}\lambda}(i\omega) (1 + \lambda \cos\theta) V_{\mathbf{q}} \frac{\partial}{\partial \omega} \frac{1}{\epsilon(q, i\omega)} \Big|_{k=k_F}. \quad (9)$$

The irreducible polarizability [7] is $\Pi(q, \omega) \simeq \nu(1 - u/\sqrt{u^2 - 1}) + i(q/4v)/\sqrt{u^2 - 1}$. After some straightforward algebra, we obtain the renormalization factor for the Dirac quasiparticle in the $r_s \ll 1$ limit as

$$Z = 1 / \left[1 + \frac{r_s}{\pi} \left(1 + \frac{\pi}{2} \right) \right], \quad (10)$$

where we have defined the interaction parameter r_s by the ratio of the interparticle potential energy to the single-particle kinetic energy. It is interesting to note that whereas for regular 2DEG, $r_s = 2me^2/k_F\epsilon_m$ is inversely proportional to the square root of the 2D density, for graphene $r_s = e^2/v\epsilon_m$ is simply a constant ~ 0.73 (with $v \simeq 10^6 \text{ms}^{-1}$ and $\epsilon_m \simeq 3$), indicating extrinsic graphene is essentially a weakly interacting ($r_s < 1$) system. (We note in this context that ordinary metals have $r_s \simeq 3-5 > 1$, and the usual semiconductor-based 2DEG may have $r_s \sim 5-20 \gg 1$!) In the leading order of r_s , Eq. (10) is similar to the corresponding expression for regular 2DEG [11] $Z = 1 - (r_s/2\pi)(1 + \pi/2)$. Beyond the leading order of r_s , the q -integral in A has a logarithmic divergence due to the interband contribution to the polarizability. Introducing a momentum cutoff k_c of the order of inverse lattice spacing, we find the corresponding logarithmic correction $\sim r_s^2 \ln(k_c/k_F)$ appears in the second order of r_s in the denominator of Eq. (10).

For quasiparticles with regular quadratic spectrum, it is well-known [9] that electron-electron interaction gives rise to effective mass renormalization of the Fermi liquid. In contrast, as the Dirac quasiparticle in graphene is massless, we have, instead, a renormalization of the quasiparticle velocity. We proceed to calculate the effective velocity renormalization below, which is defined through $v/v^* = (1 - A)/(1 + B)$, where B is the derivative of the real part of the retarded self-energy with respect to momentum k and is obtained from Eq. (8) by replacing $\partial/\partial \varepsilon \rightarrow (1/v)\partial/\partial k$. Decomposing the expression for B into line and pole contributions and taking the analytic continuation $ik_n \rightarrow \varepsilon + i0^+$, we find that the pole contribution vanishes and the expression for B becomes

$$B = -\frac{1}{2v} \text{Re} \sum_{\mathbf{q}, \lambda} \int_0^{\infty} \frac{d\omega}{\pi} \frac{\partial}{\partial k} [G_{\mathbf{k}+\mathbf{q}\lambda}(ik_n + i\omega) (1 + \lambda \cos\theta) V_{\mathbf{q}}/\epsilon(q, i\omega)] \Big|_{k, \varepsilon=k_F, \varepsilon_F}, \quad (11)$$

The evaluation of Eq. (11) is similar to that for the renormalization factor Eq. (9), albeit more tedious. Carrying out the ω -integral by integration by parts [10], and then performing the q -integral, we obtain the renormalized velocity at the Fermi level, within logarithmic accuracy, as

$$\frac{v^*}{v} = 1 - \frac{r_s}{\pi} \left[\frac{5}{3} + \ln(r_s) \right] + \frac{r_s}{4} \ln\left(\frac{k_c}{k_F}\right). \quad (12)$$

We also note that the same result here can be obtained more simply by using the static dielectric function, consistent with the fact that the effective velocity at zero temperature in the lowest leading order in r_s is only due to contribution from the static dielectric response. The first two terms in Eq. (12) derive from the intraband contribution and are similar to the expression for the regular 2DEG [12] $m^*/m = 1 + (r_s/2\pi)[2 + \ln(r_s/4)]$ whereas the last term arises solely from the interband contribution. In addition to v^* at the Fermi level, we have evaluated v^* at the Dirac point $k = 0$: $v^*/v = 1 - r_s\{1 + (1/4)\ln[(1 + 4r_s)/4r_s] - (1/4)\ln(k_c/k_F)\}$, highlighting the fact that velocity renormalization is not uniform for the entire spectrum but is in general a function of k . The renormalized spectrum therefore exhibits a small degree of nonlinearity imposed on the bare linear spectrum.

Intrinsic graphene. The irreducible polarizability for intrinsic graphene is given by [7]

$$\Pi(q, \omega) = \frac{q^2}{4} \left[\frac{\theta(vq - \omega)}{\sqrt{v^2 q^2 - \omega^2}} + i \frac{\theta(\omega - vq)}{\sqrt{\omega^2 - v^2 q^2}} \right]. \quad (13)$$

Using Eq. (13), the on-shell quasiparticle lifetime follows from Eq. (4) as $\text{Im}\Sigma_{\mathbf{k}+}^R(\varepsilon_k) \sim \sum_{\mathbf{q}} \theta(|\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_k| - \varepsilon_q) \theta(\varepsilon_k - \varepsilon_{\mathbf{k}+\mathbf{q}})$, which vanishes identically because of phase space restrictions imposed by the θ -functions. On the other

hand, the imaginary part of the self-energy at $k = 0$ follows a linear relationship with ω , and is given by

$$\text{Im}\Sigma_{\pm}^R(k=0, \omega) = \omega f(r_s), \quad (14)$$

where

$$f(r_s) = \frac{2}{\pi^2 r_s} [\pi(1 - r_s) + \frac{8 - (\pi r_s)^2}{4\sqrt{(\pi r_s)^2 - 4}} \ln \frac{\pi r_s - \sqrt{(\pi r_s)^2 - 4}}{\pi r_s + \sqrt{(\pi r_s)^2 - 4}}]. \quad (15)$$

We emphasize that the linear relation is exact for all ω , indicating that intrinsic graphene is a marginal Fermi liquid. For arbitrary values of k we calculate $\text{Im}\Sigma_{\pm}^R(k, \omega)$ numerically, and Fig. 2 shows our calculated self-energy as a function of energy ω for various values of momentum k . The numerical result for $k = 0$ in Fig. 2 agrees precisely with the analytic result of Eq. (15), providing a consistency check. As mentioned above we have $\text{Im}\Sigma_{\pm}^R = 0$ for $\omega \leq \varepsilon_k$ because there is no phase space available for virtual interband electron-hole excitations. However, for $\omega > \varepsilon_k$ the virtual interband electron-hole excitations give rise to a finite $\text{Im}\Sigma_{\pm}^R$ (i.e. finite quasiparticle lifetime). Initially $\text{Im}\Sigma_{+}^R$ ($\text{Im}\Sigma_{-}^R$) rises sharply (slowly), and for large values of momentum they increase linearly with the same slope as that for $\text{Im}\Sigma_{\pm}^R(k=0, \omega)$ (c.f. Eq. (15)). Note that there is no plasmon contribution to the imaginary part of the self-energy for intrinsic graphene. The contribution of the interband electron-hole excitations gives rise to the linear behavior of $\text{Im}\Sigma_{\pm}^R$. However, for doped graphene the contributions of the interband electron-hole excitations is completely suppressed due to phase space restrictions at zero temperature. The contributions of the intraband virtual single-particle excitations and/or the virtual excitations of plasmons give rise to higher powers of ω (i.e. ω^2) in the imaginary part of the self-energy in the doped case, which restores the usual Fermi liquid behaviour. Thus, the *qualitative* difference between intrinsic ($\text{Im}\Sigma \sim \omega$) and extrinsic ($\text{Im}\Sigma \sim \omega^2$) graphene can be *completely* understood by noting that the intrinsic system is an *insulator* (albeit a zero-gap semiconductor with no intraband single-particle excitation) and the extrinsic case has a Fermi surface with intraband single-particle excitations. Thus, any doping of graphene (intentional or unintentional) will immediately suppress its marginal Fermi liquid intrinsic character, converting it to a regular 2D Fermi liquid.

The renormalization factor can be obtained from Eq. (9), whereupon evaluating we find that $A \sim \int_0 dq/q$ diverges logarithmically, which is due to the unscreened nature of the Coulomb potential (the same divergence occurs for the exchange energy of a regular 2DEG). Therefore the renormalization factor $Z = 0$, showing that as doping goes to zero, the magnitude of the step at

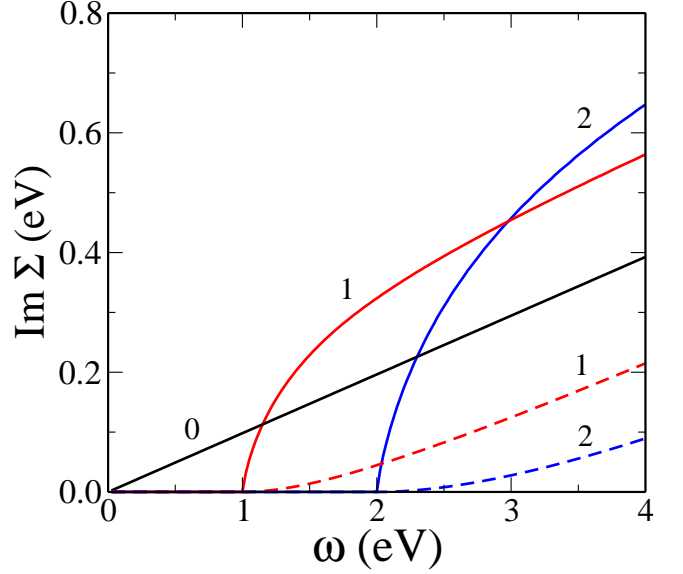


FIG. 2: (Color online) Imaginary part of the self-energy for the intrinsic graphene, $\text{Im}\Sigma_{+}^R(k, \omega)$ (solid lines), $\text{Im}\Sigma_{-}^R(k, \omega)$ (dashed lines), for different values of momentum, $k = 0, 1, 2$ eV/ $\hbar v$ (black line ‘0’, red line ‘1’, blue line ‘2’, respectively). Note that for $k = 0$, $\text{Im}\Sigma_{+}^R = \text{Im}\Sigma_{-}^R$.

the Fermi energy $\varepsilon = 0$ also shrinks to zero, approaching the Dirac point where the notion of a “Fermi surface” no longer applies, the quintessential behaviour of a marginal Fermi liquid. Using the Kramers-Kronig relations and from the fact that $\text{Im}\Sigma_{+}^R(k=0, \omega) \sim \omega$, we have $\text{Re}\Sigma_{+}^R(k=0, \omega) \sim \omega \ln \omega$, and the renormalization factor $Z \sim 1/\ln \omega$, which approaches zero logarithmically as $\omega \rightarrow 0$ at the Fermi energy. Moreover, the spectral function $\rho(k=0, \omega) = \text{Im}\Sigma_{+}^R(k=0, \omega) / \{[\text{Im}\Sigma_{+}^R(k=0, \omega)]^2 + [\omega - \text{Re}\Sigma_{+}^R(k=0, \omega)]^2\}$ diverges as $\rho(k=0, \omega) \sim 1/\omega (\ln \omega)^2$. In addition, we also find that the effective velocity $v^*/v = 1 + (r_s^*/4) \ln(k_c/k_F)$ (here $r_s^* = r_s / (1 + \pi r_s/2)$ is the renormalized interaction parameter) diverges as doping $k_F \rightarrow 0$. These results for the intrinsic graphene are consistent with Ref. [6], where the renormalization group approach is used to arrive at a similar conclusion. We note in passing that the case for a purely undoped 3D system with a gapless linear energy dispersion was considered in Ref. [13], and was found to exhibit marginal Fermi liquid behavior with a logarithmic energy dependence in $\text{Re}\Sigma$ comparable to our results for intrinsic graphene.

In conclusion, we have presented a calculation, formally exact in the $r_s \ll 1$ limit, for the renormalized Fermi liquid parameters for both extrinsic and intrinsic graphene. We find that for extrinsic graphene the analytical results for the quasiparticle lifetime, renormalization factor and effective velocity show no deviation from the usual Fermi liquid behaviour, and the Fermi liquid description is robust. On the other hand, with precise

zero doping, intrinsic graphene exhibits a quasiparticle lifetime linear in the excitation energy and a zero renormalization factor, indicating that the Fermi liquid description is marginal at the Dirac point. With a finite Fermi energy in the extrinsic graphene, the interband single-particle excitations which give rise to the linear ω -dependence of the quasiparticle lifetime (and hence the marginal Fermi liquid behavior) in the intrinsic graphene are suppressed, bringing the system back to a usual Fermi liquid. Since some finite doping is invariable in real systems, we predict real 2D graphene to be generically a Fermi liquid.

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